HIGH-RESOLUTION INFRARED SPECTROSCOPY SLIT-JET COOLED HYDROXYMETHYL RADICAL (CH_2OH): CH SYMMETRIC STRETCHING MODE

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Hydroxymethyl radical (CH_2OH) plays an important role in combustion and environmental chemistry as a reactive intermediate. Reisler's group published[a] the first rotationally resolved spectroscopy of CH_2OH with determined band origins for fundamental CH symmetric stretch state, CH asymmetric stretch state and OH stretch state, respectively. Here CH_2OH was first studied via sub-Doppler infrared spectroscopy in a slit-jet supersonic discharge expansion source. Rotationally resolved direct absorption spectra in the CH symmetric stretching mode were recorded. As a result of the low rotational temperature and sub-Doppler linewidths, the tunneling splittings due to the large amplitude of COH torsion slightly complicate the spectra. Each of the ground vibration state and the CH symmetric stretch state includes two levels. One level, with a 3:1 nuclear spin statistic ratio for K_a=0^+/K_a=1^+, is labeled as "+". The other tunneling level, labeled as "-", has K_a=0^-/K_a=1^- states with 1:3 nuclear spin statistics. Except for the K_a=$0^+ \leftarrow 0^+$ band published before [b], more bands (K_a=$1^+ \leftarrow 1^+$, K_a=$0^- \leftarrow 0^-$ and K_a=$1^- \leftarrow 1^-$) were identified. The assigned transitions were fit to a Watson A-reduced symmetric top Hamiltonian to improve the accuracy of the band origin of CH symmetric state. The rotational parameters for both ground and CH symmetric stretch state were well determined.

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[a] L. Feng, J. Wei and H. Reisler, J. Phys. Chem. A, Vol. 108.

[b] M. A. Roberts, E. N. Sharp-Williams and D. J. Nesbitt, J. Phys. Chem. A 2013, 117, 7042-7049